

Broad
Search

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 08:15:49 ON 20 OCT 2004

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STRUCTURE FILE UPDATES: 19 OCT 2004 HIGHEST RN 765878-56-6

DICTIONARY FILE UPDATES: 19 OCT 2004 HIGHEST RN 765878-56-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

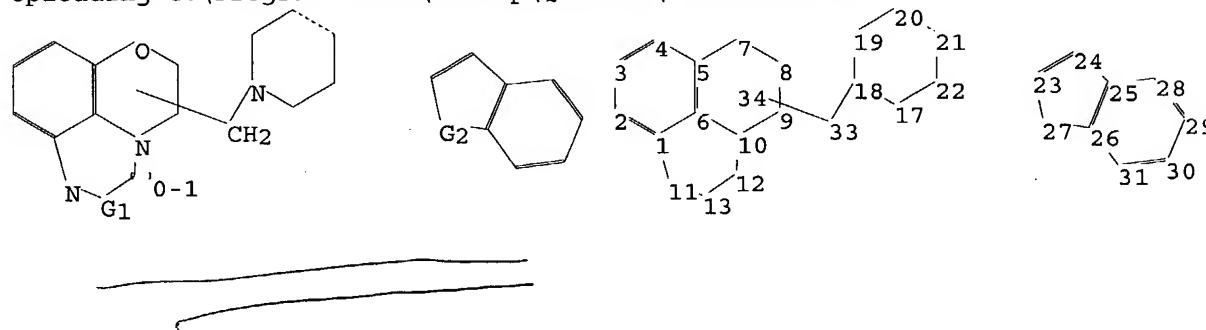
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10659531b.str



chain nodes :

33

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 17 18 19 20 21 22 23 24 25 26
27 28 29 30 31

chain bonds :

18-33

ring bonds :

1-2 1-6 1-11 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 10-12 11-13 12-13
17-18 17-22 18-19 19-20 20-21 21-22 23-27 23-24 24-25 25-26 25-28 26-27
26-31 28-29 29-30 30-31

exact/norm bonds :

1-11 5-7 6-10 7-8 8-9 9-10 10-12 11-13 12-13 17-18 17-22 18-19 18-33
19-20 20-21 21-22 23-27 23-24 24-25 26-27

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-28 26-31 28-29 29-30 30-31

isolated ring systems :

containing 1 : 23 :

G1:C,S

G2:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
33:CLASS 34:CLASS

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 08:16:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 168 TO ITERATE

100.0% PROCESSED 168 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2583 TO 4137
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 08:16:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3246 TO ITERATE

100.0% PROCESSED 3246 ITERATIONS 10 ANSWERS
SEARCH TIME: 00.00.01

L3 10 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.42	155.63

FILE 'CAPLUS' ENTERED AT 08:16:34 ON 20 OCT 2004
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FILE COVERS 1907 - 20 Oct 2004 VOL 141 ISS 17
FILE LAST UPDATED: 19 Oct 2004 (20041019/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l3

L4 1 L3

=> d ibib abs hitstr tot

Own
work

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS ON STN

ACCESSION NUMBER: 2004:252520 CAPLUS

DOCUMENT NUMBER: 140:287399

TITLE: Preparation of antidepressant azaheterocyclylmethyl derivatives of 4,5-dihydroimidazo[1,5,4-de][1,4]benzoxazine

INVENTOR(S): Gao, Hong; Stack, Gary Paul

PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA

SOURCE: PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

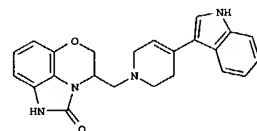
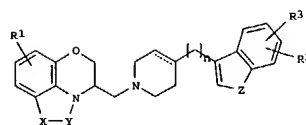
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004127493	A1	20040701	US 2003-659531	20030910
PRIORITY APPLN. INFO.: US 2002-110074 P 20020912				
US 2003-659531 A 20030910				

OTHER SOURCE(S): MARPAT 140:287399
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L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS ON STN (Continued)

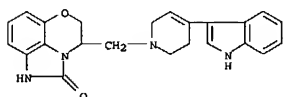


AB The title compds. [I; XY = N:CR₄, NHCO, NHCOC, NHCS, NHSO₂; Z = O, S, NRS
(wherein R₅ = H, alkyl; R₁-R₃ = H, OH, halo, CN, etc.; R₄ = H, halo, (un)substituted NH₂; n = 0-2], useful for the treatment of depression (including but not limited to major depressive disorder, childhood depression and dysthymia), anxiety, panic disorder, post-traumatic stress disorder, premenstrual dysphoric disorder (also known as premenstrual syndrome), attention deficit disorder (with and without hyperactivity), obsessive compulsive disorder, social anxiety disorder, generalized anxiety disorder, obesity, eating disorders such as anorexia nervosa and bulimia nervosa, vasomotor flushing, cocaine and alc. addiction, sexual dysfunction and related illnesses, were prepared. Thus, reacting (2-oxo-1,2,4,5-tetrahydroimidazo[1,5,4-de][1,4]benzoxazin-4-yl)methyl 4-methylbenzenesulfonate (preparation given) with 3-(1,2,3,6-tetrahydropyridin-4-yl)-1H-indole in DMSO afforded II. The biol. data such as 5-HT transporter affinity, 5-HT_{1A} receptor affinity, and antagonist activity at 5-HT_{1A} receptors, were given. The pharmaceutical composition comprising the compound I was claimed.

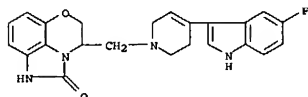
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675825-88-4P 675825-89-5P 675825-90-6P
675825-91-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of antidepressant azaheterocyclylmethyl deriva. of 4,5-dihydroimidazo[1,5,4-de][1,4]benzoxazine)

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS ON STN (Continued)

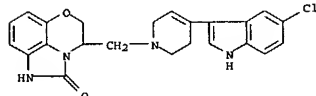
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CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,
4-[[3,6-dihydro-4-(1H-indol-3-yl)-
1-(2H-pyridinyl)methyl]-4,5-dihydro- (9CI) (CA INDEX NAME)

RN 675825-83-9 CAPLUS

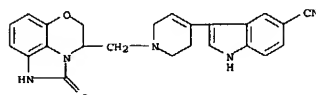
CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,
4-[[4-(5-fluoro-1H-indol-3-yl)-
3,6-dihydro-1(2H)-pyridinyl)methyl]-4,5-dihydro- (9CI) (CA INDEX NAME)

RN 675825-84-0 CAPLUS

CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,
4-[[4-(5-chloro-1H-indol-3-yl)-
3,6-dihydro-1(2H)-pyridinyl)methyl]-4,5-dihydro- (9CI) (CA INDEX NAME)

RN 675825-85-1 CAPLUS

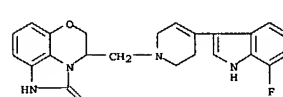
CN 1H-indole-5-carbonitrile, 3-[1,2,3,6-tetrahydro-1-[(1,2,4,5-tetrahydro-2-oxoimidazo[1,5,4-de][1,4]benzoxazin-4-yl)methyl]-4-pyridinyl]- (9CI) (CA INDEX NAME)



Habe

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS ON STN (Continued)

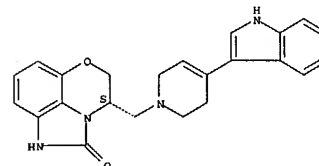
RN 675825-86-2 CAPLUS

CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,
4-[[4-(7-fluoro-1H-indol-3-yl)-
3,6-dihydro-1(2H)-pyridinyl)methyl]-4,5-dihydro- (9CI) (CA INDEX NAME)

RN 675825-95-3 CAPLUS

CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,
4-[[4-(5-fluoro-1H-indol-3-yl)-
3,6-dihydro-1(2H)-pyridinyl)methyl]-4,5-dihydro-, (4S)- (9CI) (CA INDEX NAME)

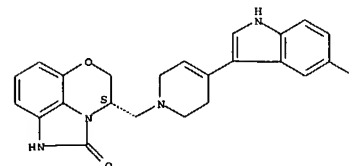
Absolute stereochemistry.



RN 675825-96-4 CAPLUS

CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,
4-[[4-(5-fluoro-1H-indol-3-yl)-
3,6-dihydro-1(2H)-pyridinyl)methyl]-4,5-dihydro-, (4S)- (9CI) (CA INDEX NAME)

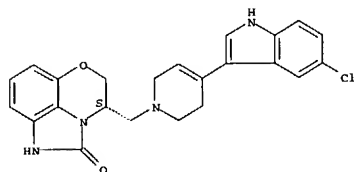
Absolute stereochemistry.



10/20/2004

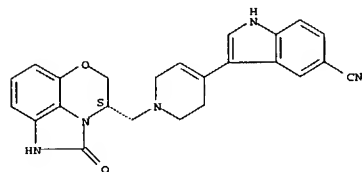
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
 RN 675825-97-5 CAPLUS
 CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,
 4-[[4-(5-chloro-1H-indol-3-yl)-
 3,6-dihydro-1(2H)-pyridinyl]methyl]-4,5-dihydro-, (4S)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.



RN 675825-98-6 CAPLUS
 CN 1H-indole-5-carbonitrile, 3-[1,2,3,6-tetrahydro-1-[[[4S]-1,2,4,5-
 tetrahydro-2-oxoimidazo[1,5,4-de][1,4]benzoxazin-4-yl]methyl]-4-pyridinyl]-
 (9CI) (CA INDEX NAME)

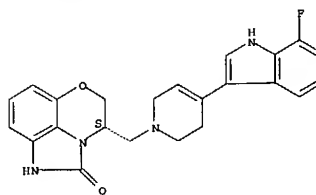
Absolute stereochemistry.



RN 675825-99-7 CAPLUS
 CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,
 4-[[4-(7-fluoro-1H-indol-3-yl)-
 3,6-dihydro-1(2H)-pyridinyl]methyl]-4,5-dihydro-, (4S)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
 FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

G1:C,S

G2:O,S,N

Match level :

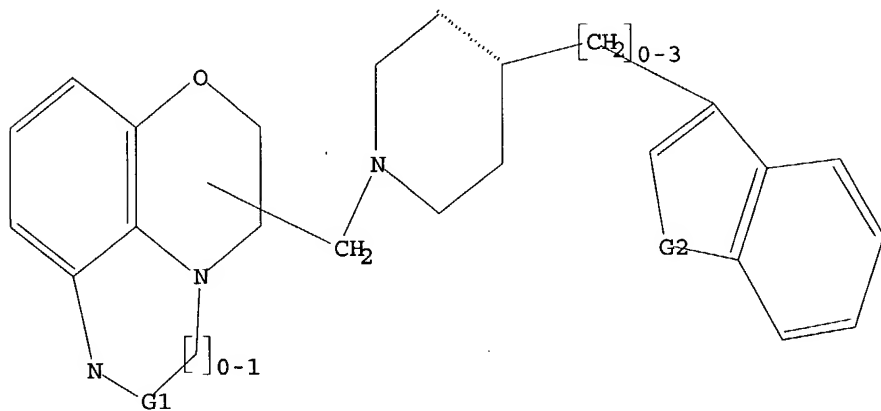
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11:Atom 12:Atom 13:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
33:CLASS 34:CLASS 37:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 C,S

G2 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 08:10:30 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 6 TO ITERATE

100.0% PROCESSED 6 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 6 TO 266
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 08:10:38 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 162 TO ITERATE

100.0% PROCESSED 162 ITERATIONS
SEARCH TIME: 00.00.01

10 ANSWERS

L3 10 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

155.42

155.63

FILE 'CAPLUS' ENTERED AT 08:10:44 ON 20 OCT 2004

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FILE COVERS 1907 - 20 Oct 2004 VOL 141 ISS 17

FILE LAST UPDATED: 19 Oct 2004 (20041019/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 1 L3

=> d ibib abs hitstr tot

Own
work

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:252530 CAPLUS

DOCUMENT NUMBER: 140:287399

TITLE: Preparation of antidepressant azaheterocyclymethyl derivatives of 4,5-dihydroimidazo[1,5,4-de][1,4]benzoxazine

INVENTOR(S): Gao, Hong; Stack, Gary Paul

PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA

SOURCE: PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

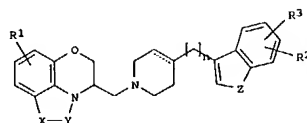
PATENT INFORMATION:

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RW: GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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US 2003-659531 A 20030910				

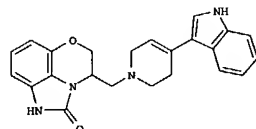
OTHER SOURCE(S): MARPAT 140:287399
GI

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

(Continued)



I



II

AB The title compds. [I; XY = N:CR4, NHCO, NHCOCO, NHCS, NHSO2; Z = O, S,

NR5

(wherein R5 = H, alkyl); R1-R3 = H, OH, halo, CN, etc.; R4 = H, halo, (un)substituted NH2; n = 0-2], useful for the treatment of depression (including but not limited to major depressive disorder, childhood depression and dysthymia), anxiety, panic disorder, post-traumatic stress disorder, premenstrual dysphoric disorder (also known as premenstrual syndrome), attention deficit disorder (with and without hyperactivity), obsessive compulsive disorder, social anxiety disorder, generalized anxiety disorder, obesity, eating disorders such as anorexia nervosa and bulimia nervosa, vasomotor flushing, cocaine and alc. addiction, sexual dysfunction and related illnesses, were prepared. Thus, reacting (2-oxo-1,2,4,5-tetrahydroimidazo[1,5,4-de][1,4]benzoxazin-4-yl)methyl 4-methylbenzenesulfonate (preparation given) with

3-(1,2,3,6-tetrahydropyridin-4-yl)-1H-indole in DMSO afforded II. The biol. data such as 5-HT transporter affinity, 5-HT1A receptor affinity, and antagonist activity

at

5-HT1A receptors, were given. The pharmaceutical composition comprising the compound I was claimed.

IT

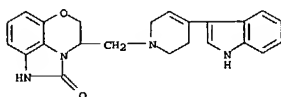
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675825-96-4P 675825-97-5P 675825-98-6P
675825-99-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of antidepressant azaheterocyclymethyl deriva. of 4,5-dihydroimidazo[1,5,4-de][1,4]benzoxazine)

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 675825-82-8 CAPLUS

CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,

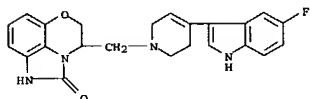
4-[[[3,6-dihydro-4-(1H-indol-3-yl)-1(2H)-pyridinyl]methyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 675825-83-9 CAPLUS

CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,

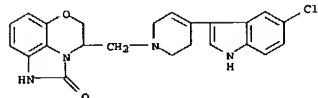
4-[[[4-(5-fluoro-1H-indol-3-yl)-3,6-dihydro-1(2H)-pyridinyl]methyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 675825-84-0 CAPLUS

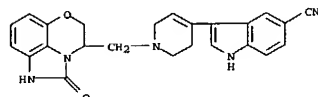
CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,

4-[[[4-(5-chloro-1H-indol-3-yl)-3,6-dihydro-1(2H)-pyridinyl]methyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 675825-85-1 CAPLUS

CN 1H-Indole-5-carbonitrile, 3-[1,2,3,6-tetrahydro-1-[(1,2,4,5-tetrahydro-2-oxoimidazo[1,5,4-de][1,4]benzoxazin-4-yl)methyl]-4-pyridinyl]- (9CI) (CA INDEX NAME)



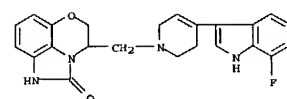
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L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 675825-86-2 CAPLUS

CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,

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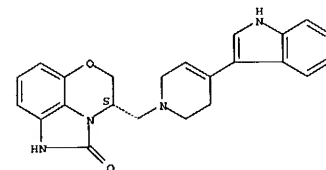


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CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,

4-[[[3,6-dihydro-4-(1H-indol-3-yl)-1(2H)-pyridinyl]methyl]-4,5-dihydro-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

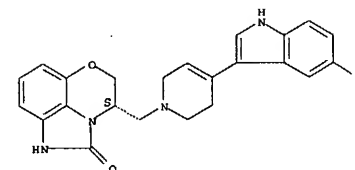


RN 675825-96-4 CAPLUS

CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,

4-[[[4-(5-fluoro-1H-indol-3-yl)-3,6-dihydro-1(2H)-pyridinyl]methyl]-4,5-dihydro-, (4S)- (9CI) (CA INDEX NAME)

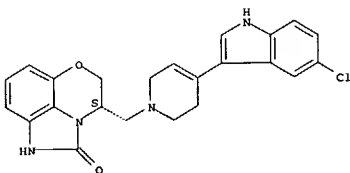
Absolute stereochemistry.



10/20/2004

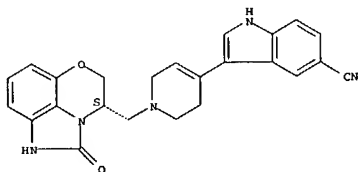
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
 RN 675825-97-5 CAPLUS
 CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,
 4-[[4-(5-chloro-1H-indol-3-yl)-
 3,6-dihydro-1(2H)-pyridinyl]methyl]-4,5-dihydro-, (4S)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.



RN 675825-98-6 CAPLUS
 CN 1H-Indole-5-carbonitrile, 3-[(1,2,3,6-tetrahydro-1-[[[(4S)-1,2,4,5-
 tetrahydro-2-oxoimidazo[1,5,4-de][1,4]benzoxazin-4-yl]methyl]-4-pyridinyl]-
 (9CI) (CA INDEX NAME)

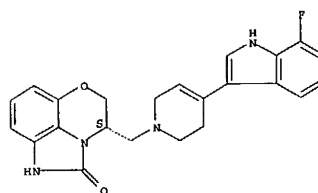
Absolute stereochemistry.



RN 675825-99-7 CAPLUS
 CN Imidazo[1,5,4-de][1,4]benzoxazin-2(1H)-one,
 4-[[4-(7-fluoro-1H-indol-3-yl)-
 3,6-dihydro-1(2H)-pyridinyl]methyl]-4,5-dihydro-, (4S)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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